

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.03 days

Global applicability domain: Outside

Local applicability domain index: 2.70e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>5-Methylindan</div> <div>Measured: 4.93</div> <div>Predicted: 2.25</div>	<div>Image not found</div> <div>9-Ethyl-9H-fluorene</div> <div>Measured: 2330</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>1H-Indene, 2-methyl-</div> <div>Measured: 12.5</div> <div>Predicted: 2.48</div>
<div>Image not found</div> <div>4-Methylindan</div> <div>Measured: 4.93</div> <div>Predicted: 2.31</div>	<div>Image not found</div> <div>3-Methylindene</div> <div>Measured: 12.5</div> <div>Predicted: 2.76</div>	